Science Communication: Writing About Solar Research for Different Audiences

Undergraduate Research Thesis

Presented in Partial Fulfillment of the Requirements for graduation "with Honors Research Distinction in English" in the undergraduate colleges of The Ohio State University

by
Brittany Trang

The Ohio State University
May 2017

Project Advisor: Professor Jonathan Buehl, Department of English

Science Communication: Writing About Solar Research for Different Audiences

Introduction

This thesis is a portfolio of science-writing documents accommodating the content of my honors undergraduate chemistry thesis ("An Indium Tin Oxide-Compatible Organic Dye for p-Type Dye-Sensitized Solar Cells") for different audiences in different genres.

This portfolio consists of the following documents:

- a press release (as would be written by an institution's research communications office for a site such as EurekAlert),
- a magazine article (as would be written by a scientific journalist for a magazine such as *Scientific American*),
- a grant proposal (as would be written by a research group/principal investigator for a grant from the National Science Foundation),
- and a graphical abstract, also known as a "Table of Contents (TOC) image" (as would be designed by a researcher for an article appearing in the *Journal of the American Chemical Society*).

I wanted to write this thesis because 1) the idea of writing a thesis in each of my majors and tying them together sounded like a fun idea (at least in the beginning!), 2) I am not sure what I would like to do as a career, and 3) I am interested in learning how to write effectively for different audiences within different genres.

I think that I would like to be a scientific researcher. However, as I have progressed through my undergrad degree, I have found that I also enjoy writing about science and editing scientific articles. I think I would be interested in a career as a research development officer, a research communications officer, an editor of a scientific journal, or a scientific journalist. Through this thesis, I got to explore writing genres from almost all of those professions. I am excited to have a portfolio of work I can show future employers, should I choose to go into a scientific-writing-related field.

I have been writing about science throughout my undergrad career—everything from editing my labmates' journal article manuscripts to re-writing the content of the Wu research group website to oral and poster presentations to applications for funding and fellowships. I've gained some formal training in technical writing though taking Dr. Buehl's English 3405 class, Special Topics in Professional Communication: Writing about Science. I am currently enrolled in English 3305, another technical writing course, and am also concurrently working on writing my chemistry thesis.

I am passionate about showing scientists that knowing how to write effectively about one's own research can reap many benefits. Similarly, from a writer's perspective, I find it interesting to see how the same subject matter can take so many different forms depending on what audience and

genre the piece is intended for. In this portfolio, I have included pieces written for the press (press release), the public (magazine article), funding agencies (grant proposal), and technical audiences (graphical abstract/TOC image).

I began each piece in this thesis by "genre norming": looking at published examples of documents in each genre to understand the genre. I looked at the rhetorical moves the writers make, the audience, the document's purpose, and the general word count. I also used handbooks and guidelines from professional publications (if available) to guide my writing.

Each piece talks about different aspects of the research depending on its purpose, whether it's persuading the audience that they should give money toward the project or informing the audience that an exciting new technology has been discovered. Each piece explains the science at a different level, whether it is making easy-to-understand analogies for people with no scientific training or delving into fine scientific detail for experts in the field.

As a final note, I would like to acknowledge that this portfolio is an exercise in science writing and not meant to be representative of actual fact. Though the science described throughout this thesis is real, there are still some results that I have not yet obtained that I have made up for the purposes of this project. Additionally, the grant proposal's project differs slightly from the project described in the other documents because it is written as if it were earlier in the research process when applying for a grant would make sense. Thus, it contains old ideas that have since been tested and changed, and it also describes the lab group members as they were approximately a year and a half ago.

—

Acknowledgements

I would like to thank Dr. Jonathan Buehl, Dr. Angus Fletcher, and Dr. Christopher Otter for agreeing to serve on my thesis committee. I have thoroughly enjoyed all of your classes and am excited that you've agreed to lend your expertise to this project.

I would also like to thank my chemistry research advisor, Dr. Yiying Wu, for supporting me through my undergraduate research career and letting my explore so many opportunities in science writing based on Wu lab research. Additionally, I would not be where I am today without (Dr.) Kevin Click. Thank you for answering my many questions and making sure I don't accidentally set myself on fire.

Lastly, I would especially like to thank my advisor, Dr. Buehl, for being supportive of my crazy second thesis idea from when I came up with the idea two years ago until now. Thank you for the endless meetings and feedback you've provided and for digging into the science with me.

Press Release: “New dye enables high-efficiency indium tin oxide dye-sensitized solar cells”

Institutions’ offices of Public Affairs or Research Communications will write press releases to promote their researchers’ work. The Hubble Space Telescope’s website gives a good description of a scientific press release.

> *“Press releases” are one of the main vehicles used by a communication office to inform the world about scientific advances…Although the main target group for press releases is the press, press releases do reach further. Press releases communicate important information to decision-makers, other mediators, scientists and even to the public. It is critically important always to tailor the style, level and content of a press release to suit the needs of the press and not the secondary target groups mentioned. (Guttridge 1)*

I began norming press releases by looking at three examples of recent materials research press releases on EurekAlert, a popular site for science news hosted by the American Association for the Advancement of Science (AAAS). Two of the press releases were around 400 words in length; the other was around 540 words in length. After examining the structure and language in the example releases, I came up with a rough structure of the press release:

> 1 sentence about broad topic
> 2 sentences about state of field/problem at hand
> 1 sentence intro to specific topic
> 2 sentences about advantages of topic presented
>
> 1 sentence: intro to study, who did it, how it fits
> 1 sentence describing system of interest
> 2 sentences describing methodology
>
> 1 sentence: description of experiment
> 2 sentences: description of result/comparison to other technologies/explanation in plainer language
> 2 sentences: more results that probably only scientists would be interested in
>
> 1 sentence: description of device study
> 1 sentence: device study results
> 1 sentence: further results/conclusions
>
> 1 sentence: this technology meets its goals and is an improvement over current technologies
>
> (around 400 words)

After discussing my drafts with Dr. Buehl, we decided to deviate from the strict structure to add more background. Including more explanations allowed me to communicate the point of the research more effectively with a lay audience. Ensuring that other understand (and feel like they understand!) the importance of the work is an essential part of the press release.

Resources:

Guttridge, Nicola. “Press release guidelines for scientists.” *Hubble Space Telescope,* www.spacetelescope.org/about_us/scientist_guidelines/. Accessed 6 April 2017.

Press releases used for norming:

Rice University. *Carbon dots dash toward 'green' recycling role*. EurekAlert, 6 December 2016. https://www.eurekalert.org/pub_releases/2016-12/ru-cdd121616.php. Web. 9 April 2017.

ICFO-The Institute of Photonic Sciences. *An invisible electrode.* EurekAlert. 19 December 2016. https://www.eurekalert.org/pub_releases/2016-12/iiop-aie121916.php. Web. 9 April 2017.

Osaka University. *Safe and inexpensive hydrogen production as a future energy source*. EurekAlert. 20 December 2016. https://www.eurekalert.org/pub_releases/2016-12/ou-sai122016.php. Web. 9 April 2017.

New dye enables high-efficiency indium tin oxide dye-sensitized solar cells

Dye-sensitized solar cells (DSSCs) are a promising alternative to traditional silicon solar cells because they offer low manufacturing costs with the added benefits of being lightweight and transparent.

However, DSSCs aren't widely used because of their low efficiencies. Researchers at the Ohio State University have recently developed a short-synthesis organic dye designed for new, high-efficiency photoelectrodes.

DSSCs come in two types: negative electron-conducting (n-type) and positive hole-conducting (p-type) DSSCs. These two types can be combined to create a "tandem" solar cell which has the potential to have a higher power output than either of its components. However, n-type solar cells have a far higher current output (~17 mA/cm^2) than their p-type counterparts (~8 mA/cm^2).

One of the factors keeping p-type solar cells from reaching higher currents is one of the conductive coatings in the p-type cell. The nickel oxide coating is not only inefficient at conducting charges, but it also absorbs a lot of sunlight before it reaches the electricity-producing dyes. Recently, researchers in Ohio State University's chemistry department have discovered that a more transparent, more conductive n-type semiconductor indium tin oxide (ITO) can replace nickel oxide in p-type cells.

However, ITO-based DSSCs are not yet more efficient than their nickel oxide predecessors because of the unusual electronic arrangement ITO requires the dye to have. So far, only inefficient metal-based dyes or more-efficient but difficult-to-synthesize organic dyes have been able to satisfy ITO's electronic requirements.

The researchers in the Yiying Wu group at Ohio State have developed a six-step synthesis that produces a dye capable of achieving currents of 6.1 mA/cm^{-2} and an efficiency of 4.9%, nearly doubling the record efficiency for p-type DSSCs. Calculations indicate that the new dye's nitrogen-linked thiophene structure provides additional conjugation that shifts the dye's highest occupied molecular orbital (HOMO) level enough to provide efficient hole injection into ITO's conduction band. Until now, scientists have been unable to use most organic dyes on ITO because of how positive the dyes' HOMO levels are.

The researchers fabricated solar cells with the dye using the I^-/I_3 redox couple in acetonitrile as electrolyte. The solar cells showed a remarkable stability over several weeks, which is a marked improvement over other solar cells also using organic electrolytes. Additionally, solar cells made with this six-step dye match the power efficiencies of other dyes that take twenty or thirty steps to make, presenting a breakthrough in efficiency achieved per synthetic step.

Developing a high-efficiency organic dye with a short synthesis for ITO-based solar cells represents an advancement toward highly-efficient p-type DSSCs. High-current p-DSSCs will allow researchers to form sought-after high-efficiency tandem DSSCs, advancing wearable solar technologies and building-integrated photovoltaic technologies to the market.

Magazine Article: “Solar’s Non-Crystalline, Clear Solution”

This magazine article is written roughly in the style of a *Scientific American* feature article. *Scientific American* publishes articles written for the general public or for technical readers looking to learn about fields other than their own, so the magazine avoids jargon and attempts to make science and technology accessible to all readers (Submission Guidelines 1).

The feature articles I normed against were between approximately 3000–3500 words; the *Scientific American* submission site says that the average length for a published article is 2500 – 3000 words (Submission Guidelines 2). My article falls at the lower edge of that range (approximately 2500).

In general, *Scientific American* articles explain both the science behind new technological advances as well as current issues in the field in enough detail that the reader comes away feeling well-versed in the area of the article’s subject matter. The articles that I normed against included several elements that helped achieve this depth and breadth for lay readers: 1) easily understood explanations and analogies of scientific concepts, 2) helpful pictures and schematics, and 3) some narrative elements and quotes to humanize the stories.

It is my hope that I have utilized those three strategies to produce a piece of journalism that is both compelling to read as well as informative for the non-technical reader.

Resources:

“Submission Guidelines.” *Scientific American,* 6 Apr 2017. www.scientificamerican.com/page/submission-instructions/.

Feature articles used for norming:

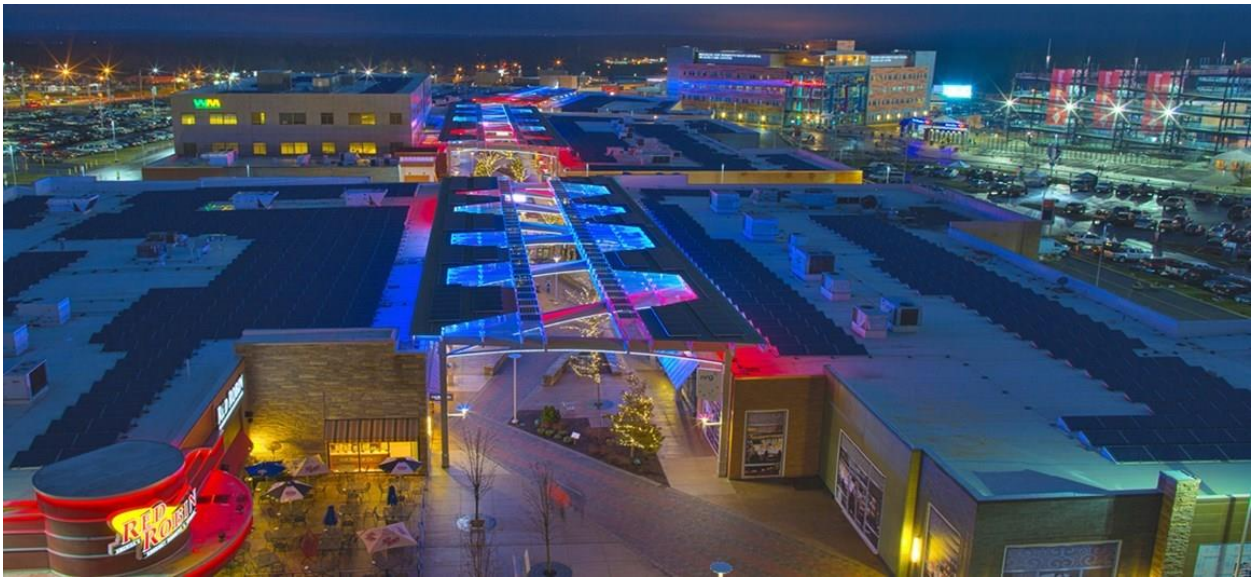
Biello, David. “Solar Wars.” Scientific American 311.5 (2014): 66–71. www.nature.com/scientificamerican/journal/v313/n1/full/scientificamerican0715-54.html. Web. 9 Apr. 2017.

Sivaram, Varun, Samuel D. Stranks, and Henry J. Snaith. “Outshining Silicon.” Scientific American 313.1 (2015): 54–59. www.nature.com/scientificamerican/journal/v311/n5/full/scientificamerican1114-66.html. Web. 9 Apr. 2017.

Solar's Non-Crystalline, Clear Solution

Abstract:
Advances in transparent solar cell technologies could mean using solar cells beyond silicon in our everyday lives.

When people think about solar panels, they usually envision roofs filled with shiny, blue-black panels. But what if solar panels could look like stained-glass windows or skylights? Because of research at the Ohio State University, transparent, colored dye-sensitized solar cells could soon replace common windows, walls, and skylights with power-producing building-integrated photovoltaics (BIPV).



The conventional photovoltaic (on rooftops, left and right) and building-integrated photovoltaic installations (center, lit) at the Patriot Place shopping center in Foxborough, Massachusetts. Photo from the DLR Group.

BIPV solar cells are different from traditional rooftop-mounted solar cells because they replace buildings' structural elements instead of being applied to the building. This new approach to solar energy could change how we incorporate clean energy into our lives.

"Think about all these windows being made out of solar cells," says Brittany Trang, an undergraduate researcher in the Yiying Wu group at the Ohio State University and lead author of a new solar cell paper in the *Journal of the American Chemical Society*. She leads me between lab benches filled with vials and water baths and glass scraps sitting in Petri dishes. It's a sunny day in Columbus, Ohio, and light streams in through the lab's floor-to-ceiling windows. She laughs. "Do they even have a LEED certification level for how efficient this place would be? This entire building is made of windows!"

The Chemical and Biomolecular Engineering and Chemistry (CBEC) building at the Ohio State University where the Wu lab is located. (courtesy of the Ohio State University Department of Chemistry and Biochemistry)

Despite the promise of BIPV, there are still wrinkles to work out before the technology can become widespread. One obstacle for BIPV solar cells is efficiency—the solar cell technologies used for BIPV are not efficient enough to compensate for their increased installation costs. But with improved technologies, that could soon change.

A popular candidate for BIPV solar technologies are dye-sensitized solar cells, the subject of Trang's new article. These solar cells are highly colored, translucent, and work well in diffuse light, which makes them perfect for replacing buildings' windows and walls.

I ask Trang what the differences are between traditional silicon solar cells, the kind you usually see on roofs, and the transparent solar cells used in BIPV.

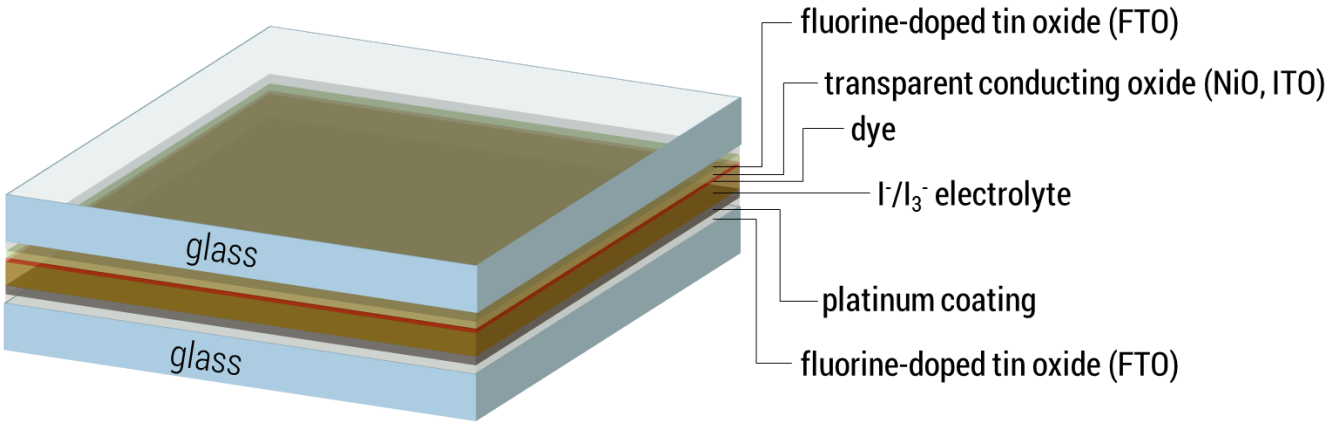
She explains that typical silicon solar cells produce electricity when the sun's photons strike one silicon layer and knock electrons free into an oppositely-charged layer, starting a flow of electrons, which we call "electric current." The dye-sensitized solar cells (DSSCs) the Wu group studies function differently. Instead of a simple positive-negative junction, DSSCs use the different electronic levels ("orbitals") within dye molecules and semiconductors to separate charges and create electricity.

Video: Silicon solar cells https://www.youtube.com/watch?v=0elhIcPVtKE
Video: Dye-sensitized solar cells https://www.youtube.com/watch?v=3KRHJSOgzcw

Watch these animations showing how silicon and dye-sensitized solar cells produce electricity.

“Think of it this way,” Trang says. “Imagine you’re moving to a third-floor apartment. If you’re the only one carrying boxes, you have to climb a lot of stairs every time you take a box up. But if you have a lot of friends, you can form a bucket-brigade system where everyone passes the boxes and no one has to walk very far. The same thing happens in a dye-sensitized solar cell—the electron gets passed through lots of different “helper” materials on its way to the other side of the circuit. This different process has distinct advantages over the silicon system.

“A lot of the problems with silicon solar cells stem from the fact that the silicon has to be defect-free for the electron to make it from one side of the other—the equivalent of you having to be really good at climbing stairs if you’re the only one,” she says. “In a dye-sensitized solar cell, we have all these helpers along the way, so we worry less about defects. In a dye-sensitized solar cell situation, you don’t have to be as good at climbing stairs since you only have to move your box up one or two stairs.”



Dye-sensitized solar cell structure

Trang opens a drawer and takes out a Petri dish with three solar cells in it. “DSSCs are like glass sandwiches,” she says, picking up one of the lab-scale solar cells. The device is constructed out of two squares of glass that have been glued onto each other. Squished in between them is a layer of brown liquid. “You have two pieces of conductive glass coated with semiconductor and dye. There’s some liquid electrolyte in between to relay the electrons from one side to the other.”

She shows me how they make the solar cells. Taking a square of glass from a paper-wrapped stack, she touches two electrical leads to the glass surface and inspects the reading on the attached multimeter. “These pieces of glass have been coated in a film that makes them conductive,” she says. She flips the glass square over. “I’m testing it to figure out which side is the conductive side.”

After noting which side of the glass is conductive, she takes out a little bottle of beige paste. “This is ITO paste,” she says, inspecting it. “We make it with indium tin oxide nanoparticles and a cellulose solution.” Using a hole-punched piece of Scotch tape as her template, she spreads the paste into a thin film on the glass to form the indium tin oxide (ITO) semiconductor layer.

“Yeah, it’s not very fancy,” she says, laughing as she peels the tape off the lab benchtop. “Science is cooler but rarely as flashy as they make it seem on TV.”

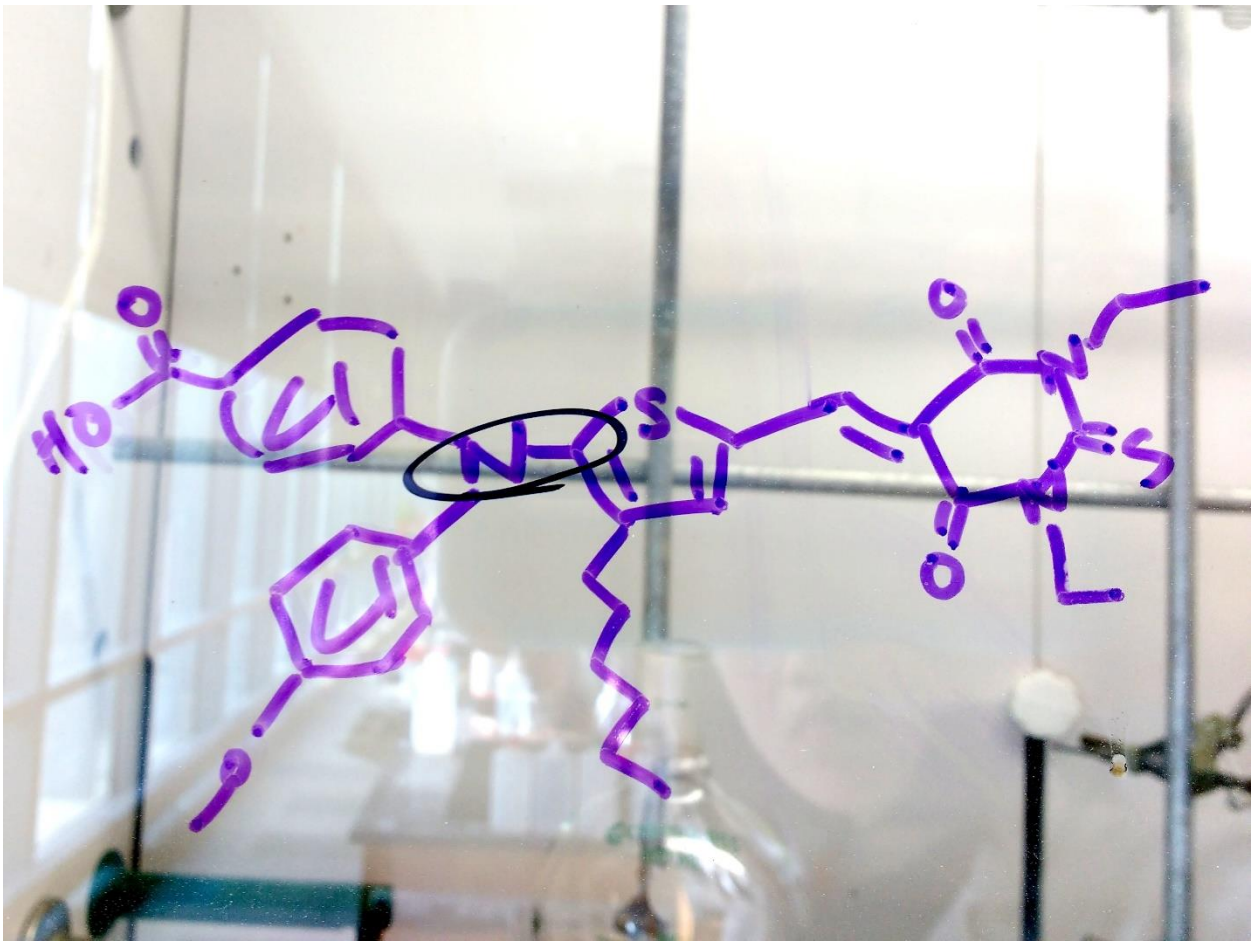
One example of the un-glamorous, behind-the-scenes sides of science is the next few steps: the film will have to be heated in an oven for a couple hours, then soaked overnight in the dye solution.

“I once heard someone say that research is 90% waiting for things to happen and 10% actually doing stuff,” Trang says as she pulls out a glass jar filled with red liquid. “It’s pretty true. And another thing that you don’t see on TV is how slow science is. It took me three years to figure out how to make this dye.”

“This dye” is the subject of the new paper, which Trang and her coworkers from the Yiying Wu group published in the *Journal of the American Chemical Society*. The paper details the short synthesis of a new dye that works on indium tin oxide-based dye-sensitized solar cells. Indium tin oxide (ITO) is a semiconductor that the Wu group hopes will replace nickel oxide as the standard semiconductor for “positive-type” (p-type) DSSCs, the under-developed and under-studied variety of DSSCs.

ITO is a faster charge conductor and absorbs much less light than nickel oxide, letting more sunlight reach the dyes beneath it. Just switching to ITO instead of NiO can help increase the efficiency of the solar cell by letting more light reach the electricity-producing dyes. There’s just one problem—a new semiconductor means different electronic levels, and ITO’s levels are different enough that new dyes need to be created for it.

“The novelty of our new dye is based on this bond,” Trang says, taking out a marker and drawing on the glass window of a nearby fume hood. She draws a molecule with an N connected to a pentagon with an “S” at one of its corners and circles the bond between the N and the pentagon. “Without it, the dye looks like this.” She holds her hands out flat in front of her, tips of her fingers touching, one hand rotated almost perpendicular to the other. “But with this bond, the dye flattens out.” She rotates her hand so they are both flat. “Making the dye planar lets the different parts of the molecule share electrons easier and moves the electronic levels the way we want them to go. The only problem is that the bond turned out to be extremely fussy, which is why it took me forever to figure out how to make it.”



The structure of Trang's dye, troublesome bond circled in black

Using ITO (indium tin oxide) as the semiconductor in p-type DSSCs is a pretty new concept. Until recently, most p-DSSCs used nickel oxide as the semiconductor that the dye anchors to and injects charge into. However, nickel oxide's sub-par conducting abilities and debatable transparency always limited the efficiency of the solar cells made with it.

The NiO or ITO semiconductors coating the glass "bread" pieces of the DSSC sandwich have a "band gap": the gap between the level the electrons usually inhabit (the "valence band") and the level where the lowest unoccupied electron states are (the "conduction band.") The band gap is like the distance between two stairs—you can stand on the first "valence" stair and use some energy to move up to the second "conduction" stair, but you can't really stand in between.

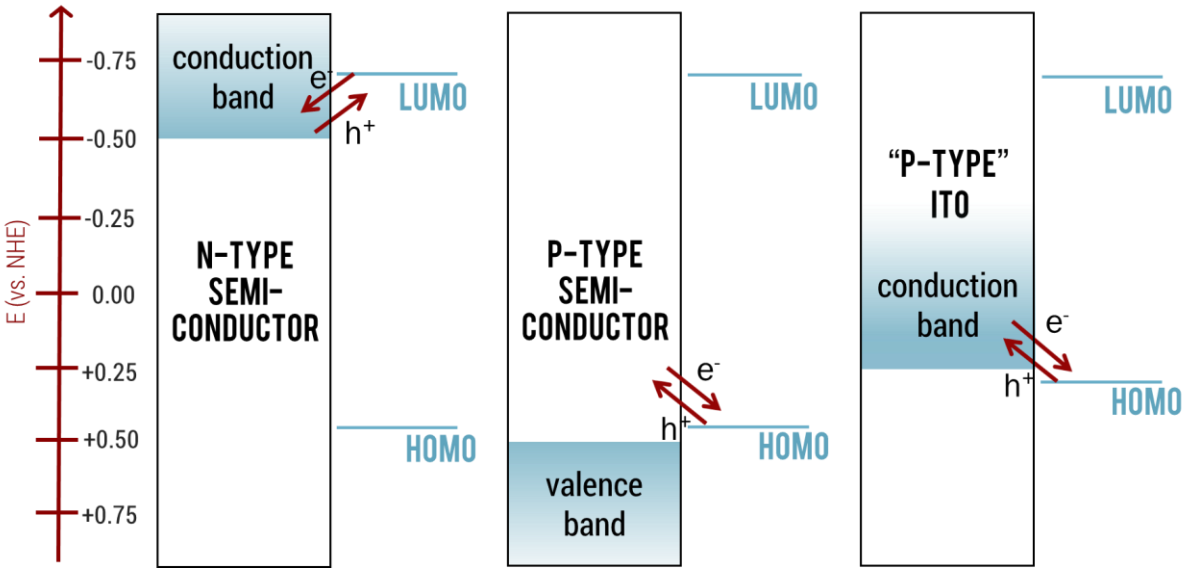
The dye molecules attached to the semiconductors have a similar electronic structure, but instead of the valence band and the conduction band, they have the HOMO (the Highest Occupied Molecular Orbital), which is occupied with electrons, and the LUMO (the Lowest Unoccupied Molecular Orbital), which is the lowest level that doesn't have electrons in it.

DSSCs create electricity (a flow of charges) by absorbing light energy from the sun, which excites an electron from the dye molecule's filled HOMO level to its empty LUMO level. After

gaining this energy from the sun, the "excited" electron then "relaxes," making its way through the solar cell and the external circuit (where the electricity is harvested) by jumping to materials with lower and lower electronic levels (like a Slinky on a staircase) as it returns back to the dye's ground-state HOMO.

Usually, negative-type (n-type) DSSCs inject excited electrons from the dye's LUMO into the semiconductor's conduction band, which is lower in energy than the LUMO. Conversely, the dyes in positive-type (p-type) DSSCs take an electron from the semiconductor's valence band (which is higher in energy than the dye's HOMO), thus injecting a positively-charged "hole" into the semiconductor where the electron once was. The "p-type" ITO approach, however, is an odd combination of both of these mechanisms—"hole injection" into ITO's conduction band—that changes the p-type DSSC game.

Two years ago, the Wu group published their discovery that ITO, a material that absorbs much less light and is a much better charge conductor, could be used in p-type DSSCs through an unusual electronic alignment: instead of injecting holes into the semiconductor's valence band, the dye injects holes into ITO's conduction band.



Electron/hole injection process for n-type, p-type, and p-type ITO DSSCs. (And yes, the numeric scale looks upside-down. The electrochemical world is weird.)

"People didn't want to believe it," says Kevin Click, a PhD candidate in the Wu lab and a co-author of the original ITO paper. "It took a long time to get published because reviewers kept sending the paper back to us. They didn't know what to do with it. They never thought it would work."

For dyes to work on ITO, they have to have an odd electronic arrangement: their HOMO levels have to be very negative, quite close to but just more positive than the ITO conduction band level. Metal-based dyes have HOMO levels close to this level, but DSSCs made with these dyes suffer from significant "dark current"—current measured in the dark when the sunlight isn't

shining on the solar cell. This current comes from processes not driven by light—like electrolyte leaking electrons into the semiconductor, producing an opposing flow of electrons that ultimately lowers the output of the solar cell.

But some dyes incorporate blocking elements that prevent dark current. Like bumpers at a kids' bowling party, these blocking chains keep the electrons where they're supposed to go. However, only organic dyes have these bulky blocking chains, and the HOMO levels of organic dyes are too far away from the ITO conduction band level to be able to interact with it.

To use an organic dye on ITO, the dye's HOMO level has to be shifted upwards. Otherwise, it's like trying the use the bucket-brigade method for moving into an apartment, but having your friends stand on completely different floors.

And that's where Trang's dye comes in. Her dye—complete with its "fussy" bond—raises the HOMO to within shooting range of the ITO conduction band and incorporates the essential blocking elements. It also has a short and sweet production process. Many other organic dyes, including another organic dye made for ITO, take up to twenty or thirty steps to make. Trang's dye only takes six.

"I'm interested in making materials that could actually be industrially manufactured," she says. "My synthesis has a long way to go before it would be easy to make this dye industrially, but it's a lot closer to showtime than a lot of other organic dyes."

Trang takes the lid off her jar of red liquid and uses tweezers to pull out a piece of glass with a dark red film. Like a cooking show, she's prepared this one ahead of time.

"So this is what it looks like after we soak it in the dye," she says, rinsing off the film with some solvent. "The dye molecules stick to the ITO film, which is why it turned red."

She assembles the rest of the cell, sealing the dyed piece of glass together with the counter-electrode, a piece of glass coated in a thin, grayish coating of platinum. With the help of a makeshift vacuum chamber, she injects the brown liquid electrolyte—a combination of an iodide salt and iodine dissolved in an acetonitrile solvent—into the solar cell through a tiny hole. She uses a tiny iron to seal the hole with a piece of heat-activated plastic. After sealing the edges with some clear nail polish, she holds it up to inspect it.

"Perfect," she says. "Now we can test it."

We walk into a room with lots of computers and wires on the benchtops. Trang clips two metal alligator clips onto the opposite sides of the solar cell, the metal teeth on the clips making contact with the conductive sides of the glass. The clips are attached to a potentiostat, an instrument that controls the electric potential of the circuit.

Trang adjusts the position of the solar cell underneath an extremely bright lamp that simulates the sun. "Try not to look directly at it," she warns me as she starts the scan. A line crawls across the screen as the potentiostat changes the voltage.

“That’s it,” she says, watching the graph of the electric current the solar cell is producing. “Three and a half years of work, packed into that tiny solar cell.” She smiles a little bit as the line grows higher and higher, climbing to a record current of 6.1 and an efficiency of 4.9%, doubling the record efficiency for p-type DSSCs.

Trang’s dye’s higher current means that the research team can start building “tandem” DSSCs, which combine n-type and p-type cells to make a solar cell with an even higher power output.

“We are excited about Brittany’s results because we can current-match the p-type side with the n-type side now,” says Professor Yiying Wu, the principal investigator of the lab. “Tandem cells are the future of the dye-sensitized solar cell. They are the ultimate goal.”

Tandem DSSCs eliminate the need for expensive platinum counter-electrodes and have two dyes that can each cover a different part of the solar spectrum. A highly-efficient tandem cell could be the breakthrough that dye-sensitized solar cells need to capture the building-integrated photovoltaic and wearable solar markets, changing how we integrate alternative energy into our lives.

Grant Proposal: “An Indium Tin Oxide-Compatible Organic Dye for p-Type Dye-Sensitized Solar Cells”

A PI (principal investigator) will write a grant proposal in order to obtain funding for their research projects. The purpose of the grant proposal is to convince the funding agencies that the research is well-thought-out, fits the goals of the program, and will succeed.

I wrote this grant to fit the guidelines of the National Science Foundation (NSF), specifically the NSF’s “Energy For Sustainability” program. This program supports research into “innovative processes for the sustainable production of electricity and fuels” and welcomes projects that “stress molecular level understanding of phenomena that directly impacts key barriers to improved system level performance (e.g. energy efficiency, product yield, process intensification).” The program also stipulates that the proposed research “research should be inspired by the need for economic and impactful conversion processes” and specifically includes support for organic photovoltaic research. The project that I am proposing fits all of the above guidelines, making this program a logical fit for this proposal.

The NSF’s Policy and Award Policies and Procedures guide specifies that the grant proposal should contain many specific sections, including:

a. Cover Sheet
b. Project Summary
c. Table of Contents
d. Project Description
e. References Cited
f. Biographical Sketch(es)
g. Budget and Budget Justification
h. Current and Pending Support
i. Facilities, Equipment and Other Resources
j. Special Information and Supplementary Documentation
  • Data Management Plan
  • Postdoctoral Mentoring Plan (if applicable)
k. Single Copy Documents
  • Collaborators & Other Affiliations Information
(NSF PAPPG 15)

I decided to write the parts of the grant that seem most relevant to the purposes of this portfolio: the parts of the proposal that deal directly with talking about the research in a persuasive manner. I have chosen to include parts b, d, and e: the one-page project summary, the up-to-fifteen-page project description, and the references cited.

The other portions of the grant—for example, the Cover Page; Budget and Budget Justification; Facilities, Equipment and Other Resources—are either standard forms or statements that can be

copied from elsewhere (Cover Page; Table of Contents; Biographical Sketch(es); Budget and Budget Justification; Facilities, Equipment and Other Resources) or are outside of the scope of this project (Budget and Budget Justification).

The guide specifies that "The Project Summary should be written in the third person, informative to other persons working in the same or related fields, and, insofar as possible, understandable to a scientifically or technically literate lay reader" (pg 18). I have tried to extend this guideline for the knowledge of the audience to the rest of the proposal.

Since this document is intended for a technical audience, it carries the most similarities to my chemistry thesis. I did borrow much of the content from my chemistry thesis, since the explanations and reasoning behind the scientific process are very similar. However, the grant proposal is a persuasive document, whereas the thesis's purpose is to explain the entire research process in detail.

I have included below an example of changing language/content in the grant proposal to be more persuasive rather than expository, as it is in my thesis. Since the grant proposal seeks to persuade others that the study is reasonable, feasible, and important, I chose to include fewer caveats to DSSC's role in the future of photovoltaics in the introduction section example.

Thesis

Solar power is the most promising renewable energy source. It's more renewable and sustainable than nuclear, more long-lived than geothermal, more efficient than biomass, more plentiful than hydro or wind, and more of it hits the Earth in one hour than the world consumes in an entire year (Lewis).

Silicon solar cells are current the industrial and commercial standard for solar energy. Over the past few years, the price of solar energy has dropped—the cost of an average US residential solar array went from $5.86 per watt in 2012 to $3.60 per watt in 2014 (Warburg). The price of utility-scale solar has also become almost comparable to coal—the estimated levelized cost for solar plants using crystalline silicon or thin film solar panels is now 7.2 to 8.6 cents/kilowatt-hour (kWh), compared to 6.5 cents/kWh for a coal plant (Warburg).

Since their invention in the 1990s, dye-sensitized solar cells (DSSCs) have been discussed as a possible alternative for silicon solar cells because they are lightweight and promise to be easier and cheaper to manufacture than silicon solar cells. However, while costs of silicon solar cells have dropped, the low efficiencies of DSSCs have not risen to meet expectations. In 1997, the efficiency for the foremost dye-sensitized solar cells was 10% (Nazeeruddin, Péchy, and Grätzel); by 2016, the record certified efficiency had only increased to 11.9% (Green et al.; Komiya R, Fukui A, Murofushi N, Koide N, Yamanaka R), a record that has stood since 2011 (Komiya R, Fukui A, Murofushi N, Koide N, Yamanaka R). In comparison, the efficiency of silicon solar cells is more than double the efficiency of DSSCs—25.6% for a crystalline silicon cell (Green et al.). While the raw material costs for dye-sensitized and organic solar cells may still be substantially cheaper than pristine crystalline silicon, their low efficiencies and short lifespans mean that it may be impossible for DSSCs to ever surmount the cost-per-unit-energy gap and compete with silicon solar cells (Kalowekamo and Baker).

While it appears unlikely that DSSCs will overtake silicon solar cells in terms of efficiency or power output, DSSCs and other organic and thin-film solar technologies have niche markets like the growing building-integrated photovoltaics (BIPV) trend in which solar cells are included as a building element in the construction of a building or structure. Wind Tower, part of the University of British Columbia's Regent College theological library, includes a glass wall embedded with solar cells (Regent College), and Patriot Place, the shopping mall next to the Patriots football team's Gillette Stadium, has integrated translucent solar cells into the canopies over the mall's walkways (Warburg). Because they are both transparent and colored, DSSCs are a highly desirable technology for BIPV.

Grant Proposal

Since their invention in the 1990s, dye-sensitized solar cells (DSSCs) have been discussed as a possible alternative for silicon solar cells because they are lightweight and promise to be easier and cheaper to manufacture than silicon solar cells. However, the low efficiencies of DSSCs have not risen according to expectations. In 1997, the efficiency for the foremost dye-sensitized solar cells was 10% (Nazeeruddin, Péchy, and Grätzel); by 2016, the record certified efficiency had only increased to 11.9% (Green et al.; Komiya R, Fukui A, Murofushi N, Koide N, Yamanaka R), a record that has stood since 2011 (Komiya R, Fukui A, Murofushi N, Koide N, Yamanaka R). By comparison, the efficiency of silicon solar cells is more than double the efficiency of DSSCs—25.6% for a crystalline silicon cell (Green et al.). Much more research is needed for DSSCs to become industrially viable.

However, DSSCs remain interesting because they are transparent, making them ideal for use in energy-generating windows, and can be roll-to-roll printed on plastic substrates, making them candidates for wearable solar cells. Even though they currently have low efficiencies, DSSCs hold promise for applications that silicon and other solar cell technologies cannot fulfill. These applications could expand the ways that we integrate clean energy generation into daily living.

I normed this grant against a successfully funded NSF grant proposal from my lab group. Though the example document was much larger and more rigorous in scope and characterization, it gave me the basic structure for the grant proposal. Knowing how the project was carried out and seeing how the work was described in the grant showed me how the actual lab work translates to the persuasive language that grant writers use.

I would like to thank Benjamin Garrett, a graduate student in the Wu group, for providing me with the funded NSF grant proposal example and thank Kevin Click for providing me with example of a funded Department of Energy (DOE) proposal.

Resources:

NSF Policy and Award Policies and Procedures Guide. NSF 17-1, National Science Foundation, 30 January 2017. www.nsf.gov/pubs/policydocs/pappg17_1/nsf17_1.pdf. 9 April 2017.

"Energy for Sustainability." National Science Foundation. www.nsf.gov/funding/pgm_summ.jsp?pims_id=505339. 9 April 2017.

An Indium Tin Oxide-Compatible Organic Dye for p-Type Dye-Sensitized Solar Cells

PROJECT OBJECTIVE: This proposal aims to study the synthesis of an nitrogen-linked-thiophene-containing dye for indium tin oxide-based (ITO-based) p-type dye-sensitized solar cells (DSSCs). The fundamental hypothesis is that by changing out the typical triphenylamine moiety for a diphenylamine linked to a thiophene, the dye's highest-occupied molecular orbital (HOMO) level will shift negatively enough in potential to interact with the ITO conduction band. By switching from the current state-of-the-art nickel oxide (NiO) semiconductor to the ITO semiconductor, we can increase the amount of photons reaching the dyes, producing high-efficiency p-type dye-sensitized solar cells.

Compared to current ruthenium dyes, the proposed dye's organic structure will allow for better dye-packing on the semiconductor, raising the dye-loading and thus the light harvesting efficiency (LHE) of the solar cells. The organic structure will also allow recombination-blocking alkyl chains to be incorporated into the dye structure, raising the overall efficiency of p-type ITO-based DSSCs.

The synthesis of this dye is also of interest, as this synthesis is short (13 steps) for an organic dye, yet is expected to yield higher currents and efficiencies than dyes with twenty- or thirty-step syntheses. The synthesis is planned to be both sustainable and scale-up ready.

Additionally, this study is expected to advance organic synthetic knowledge in the area of C – N bond formations. The crucial reaction in this synthesis is the C – N bond-forming reaction between the secondary amine and the thiophene. This bond is the subject of many reactions (Chan-Lam, Buchwald-Hartwig, Ullman) but has been relatively unexplored with this dye's cross-coupling partners, diphenylamines and thiophenes. Within this study, we plan to examine the conditions required for C – N bonds to form between secondary amines and thiophenes. The specific objectives of the proposed study are:

1. To produce an organic dye for ITO-based p-type dye-sensitized solar cells that has a short and scalable synthesis.
2. To characterize devices made with this dye and compare the performance of the ITO-based solar cells with conventional NiO-based solar cells.
3. To provide synthetic insight into the conditions necessary for C – N bonds to form between amines and thiophenes.

Intellectual Merit: The proposed project investigates whether using the N-linked thiophene motif in an organic p-type dye will shift the HOMO level of the dye sufficiently enough to allow the dye to efficiently inject holes into the ITO conduction band and create high-efficiency DSSCs. The impacts include: 1) creating an improved-efficiency dye-sensitized solar cell device 2) producing a dye that has a shorter, more sustainable synthesis process much more scale-up-ready than other dyes, 3) contributing to the understanding of cross-coupling amination reactions by examining the conditions needed for successful amine-thiophene couplings, and 4) achieving high-current p-type dye-sensitized photoelectrodes that are well-suited to current-match with n-type dye-sensitized photoelectrodes to create high-efficiency tandem DSSCs.

Broader Impacts: Developing dyes that have both an efficient performance and an efficient synthesis route will help advance DSSCs to the market. DSSCs are promising for both wearable solar and building-integrated photovoltaics (BIPV) technologies. Examining new ways to increase DSSCs' efficiency will give us new ways to produce clean, solar energy.

Additionally, this project is designed to teach both undergraduate and graduate students. An undergraduate-graduate student pair will work on this project, teaching then both basic scientific and research skills as well as leadership and mentorship skills.

BACKGROUND AND UNIQUENESS OF PROPOSED WORK

Since their invention in the 1990s, dye-sensitized solar cells (DSSCs) have been discussed as a possible alternative for silicon solar cells because they are lightweight and promise to be easier and cheaper to manufacture than silicon solar cells. However, the low efficiencies of DSSCs have not risen according to expectations. In 1997, the efficiency for the foremost dye-sensitized solar cells was 10%[1]; by 2016, the record certified efficiency had only increased to 11.9%[2,3], a record that has stood since 2011[3]. By comparison, the efficiency of silicon solar cells is more than double the efficiency of DSSCs—25.6% for a crystalline silicon cell[2]. Much more research is needed for DSSCs to become industrially viable.

However, DSSCs remain interesting because they are transparent, making them ideal for use in energy-generating windows, and can be roll-to-roll printed on plastic substrates, making them candidates for wearable solar cells. Even though they currently have low efficiencies, DSSCs hold promise for applications that silicon and other solar cell technologies cannot fulfill. These applications could expand the ways that we integrate clean energy generation into daily living.

Today's best-performing DSSCs are negative-type, or "n-type," DSSCs, which are named for the negative electrons that the dye injects into the semiconductor of these solar cells. These n-type cells have achieved efficiencies of 12.3%[4]. By contrast, positive-type, or "p-type," DSSCs (named for the positive hole the dye injects into the semiconductor by taking away an electron from the semiconductor) have only reached 2.51% efficiency[5].

Ideally, n- and p-type DSSCs would be combined together in a high-efficiency "tandem cell." In n-type and p-type DSSCs, the solar cell is composed of either a photoanode (for n-type cells) and a "dummy" platinum counter-electrode, or a photocathode (for p-type cells) and a "dummy" platinum counter-electrode. In a tandem cell, the n-type photoanode and the p-type photocathode are combined into a single cell. This design eliminates the need for the expensive, ineffective platinum counter-electrode because both the photoelectrode and the photocathode are photosensitized. This dual-photosensitization also allows for broader absorption of the solar spectrum, since the dye on one side can be tuned to absorb more on the ultraviolet side of the spectrum and the dye on the other side can be tuned to absorb on the infrared side of the spectrum.

In the tandem design, the open-circuit voltages of each side of the tandem cell add together, boosting the efficiency of the overall cell. Unfortunately, the currents produced by each side of the tandem cell are not additive—they are limited by the lowest-current-producing side of the cell. While high-performing n-type cells[4] produce currents around 17 mA/cm^2, the record p-type cells[5] only produce currents less than 8 mA/cm^2. At this point, tandem cells essentially are less efficient than n-type cells alone. However, with additional advances in p-type cell efficiencies, highly-efficient tandem DSSCs could become a reality. We want to investigate high-efficiency, high-current p-type systems so we can create efficient tandem DSSCs.

The main factor that limits p-type DSSCs' efficiencies is the nickel oxide (NiO) semiconductor used for the photocathode. NiO is currently the industry-standard semiconductor for p-type solar cells, but it limits DSSCs' efficiency because it absorbs heavily in the solar spectrum and steals light from the electricity-producing dyes (Figure 1B). Another semiconductor, indium tin oxide (ITO), is a much more suitable semiconductor for high-efficiency p-type DSSCs than nickel oxide because it does not parasitically absorb light and is much faster at transporting charge.

Changing from NiO to ITO semiconductors gives the dyes access to much more light and allows the solar cell to create more electricity more efficiently (Figure 1B.)

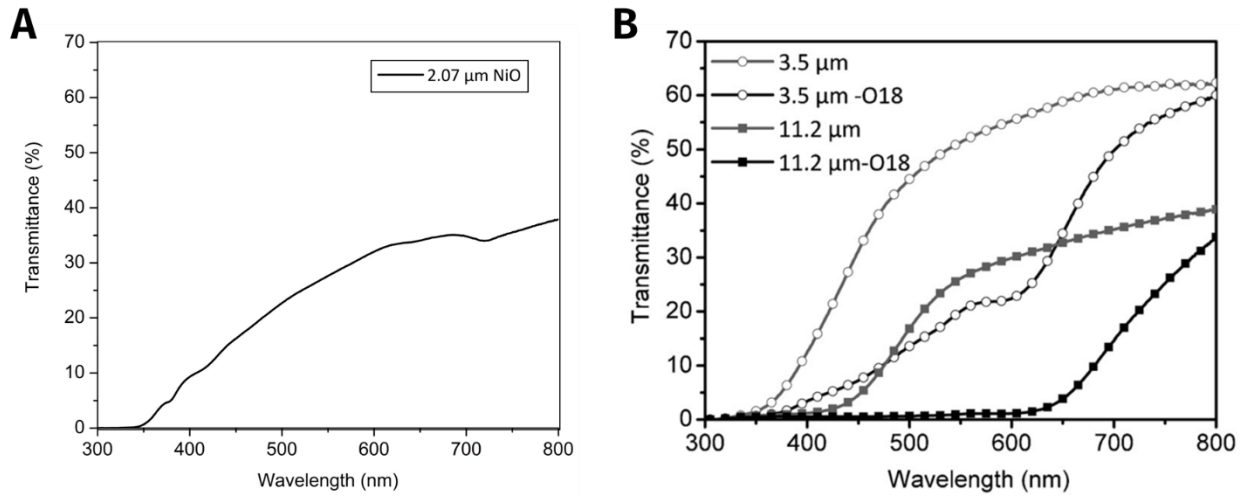


Figure 1 A) Transmittance of nickel oxide (used with permission from Bradley Schockman). B) Transmission of various thicknesses of indium tin oxide (ITO) both bare and with adsorbed O18 dye[6].

ITO normally works as an n-type semiconductor, but a recent study by our lab (Huang et al.) discovered that ITO works well in p-type cells under a specific electronic arrangement[6]. In that arrangement, instead of injecting a hole (a vacancy of an electron) from the p-type dye's highest occupied molecular orbital (HOMO) into the p-type semiconductor's valence band (VB), the p-type dye instead injects a hole into ITO's conduction band (CB). See Figure 2.

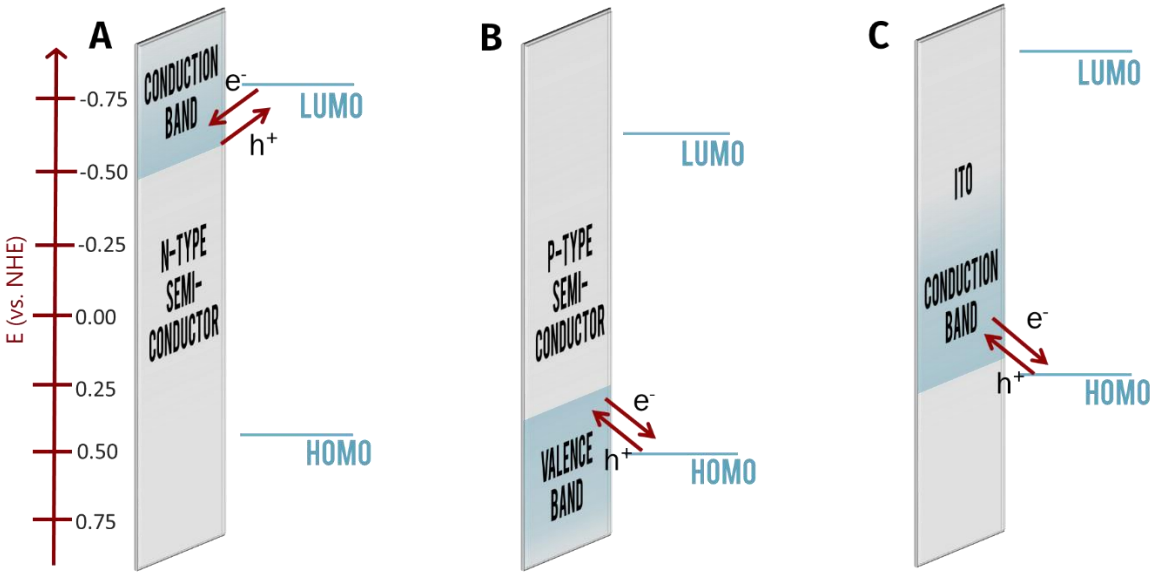


Figure 2 Electron/hole injection processes for A) n-type, B) p-type, C) "p-type" ITO dye-sensitized solar cell electrodes.

However, this shift from injecting into the more positive semiconductor VB to the more negative ITO CB means that the dye's HOMO has to become more negative so it will align with the ITO

CB and inject efficiently. Huang et al. found that the only dyes that have HOMO levels negative enough to work with "p-type" ITO are ruthenium-based dyes[6] (Figure 3).

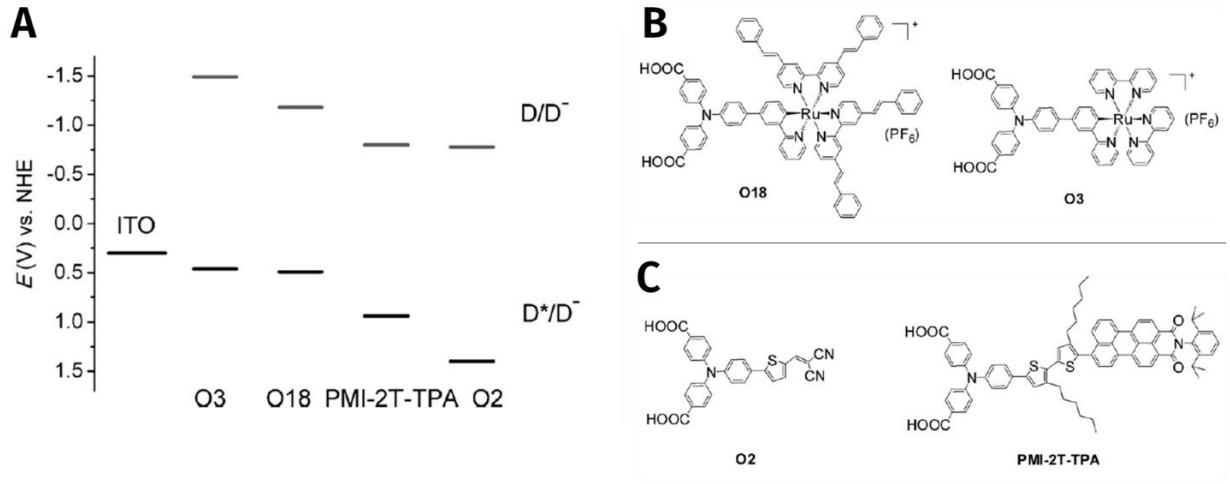


Figure 3 A) HOMO (lower) and LUMO (higher) electronic levels of various dyes in relation to the conduction band of ITO. B) Structures of ruthenium-based O18 and O3 dyes, which are compatible with ITO. C) Structures of organic dyes O2 and PMI-2T-TPA, which do not work on ITO[6].

Unfortunately, these ruthenium dyes suffer from two problems which limit solar cell efficiency: 1) significant dark current (producing current in the dark from processes that are not driven by light such as the electrolyte leaking opposing current into the semiconductor) and 2) recombination (electrons or holes in the solar cell unproductively recombining with each other instead of flowing through the circuit and producing electricity.)

To overcome the dark current problem, researchers have developed organic (non-metal-based) dyes that protect the semiconductor surface by using long, hydrophobic (water- and electrolyte-repelling) hexyl chains[7,8]; however, the organic dyes we currently have do not have negative enough HOMO levels to work with "p-type" ITO[6] (Figure 3).

Unfortunately, the two organic dyes studied by Huang et al. produced very little current in the ITO-based devices. The device made with dye **O2** even reversed direction and produced anodic current (as would be expected from an n-type system) rather than the expected cathodic current[6] because of its much more positive HOMO level, which is not able to efficiently inject holes into the ITO CB.

RESEARCH PLAN AND PRELIMINARY STUDIES

The proposed project's main focus is on designing and synthesizing a high-current, high-efficiency organic dye that has a negative enough HOMO level potential to efficiently inject holes into ITO.

To shift the HOMO level of the dye, we propose replacing the triphenylamine donor moiety common to organic p-type dyes (see, for example, dyes O2 and PMI-2T-TPA in Figure 3) with a thiophene linked to the N atom of a diphenylamine (see Fig. 4.). Additionally, the dye contains a strong, aromatizable diethylthiobarbituric electron acceptor that adds to the conjugation of the molecule, further narrowing the HOMO – LUMO gap and redshifting the absorbance of the dye[9].

As a secondary goal, we plan to increase the current and efficiency of the solar cell relative to the metal-based dyes. Including alkyl chains on the thiophene pi-bridge to stop electron recombination with the semiconductor surface will increase the IPCE and the current of the cell.

To accomplish these goals, we plan to change the third phenyl ring of the common triphenylamine donor moiety to a thiophene. In a study by Chang and Chow[10], making this change increased the planarity of the dye. The change from a phenyl to a thiophene decreases steric hindrance, allowing the pi bridge to become almost completely flat. This increases the molecule's planarity and thus the electron-sharing (conjugation) on the thiophenes. Increased conjugation leads to a decreased HOMO–LUMO gap and shifts the HOMO level negatively by over 0.2 V[10]. This decreased HOMO–LUMO gap correspondingly redshifts the dye's absorbance to the more-favorable red–infrared portion of the spectrum[10], also increasing the efficiency of the cell by increasing the amount of photons the dye can absorb.

The proposed dye structure is pictured in Figure 4. Most organic dyes for dye-sensitized solar cells have four essential components: the anchoring group, the donating group, the π-bridge, and the acceptor group[11].

The anchoring group (black), commonly a carboxylic acid, is essential because it anchors the dye to the semiconductor surface. The electron-rich donating group (blue) donates the electrons that are excited to the LUMO. The LUMO normally resides on the electron-deficient accepting group (red). The conjugated pi-bridge on this dye also includes hexyl chains (highlighted in purple) to block electrons in the electrolyte from recombining with the semiconductor surface.

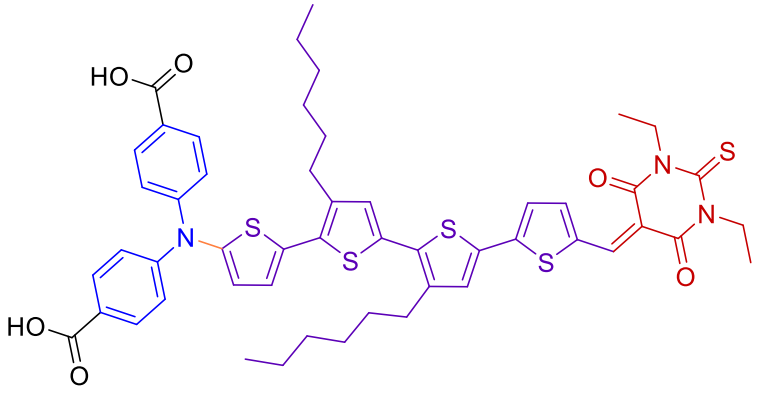


Figure 4. Dye structure. The dye consists of two carboxylic acids (black) as anchoring groups to bind the dye to the nickel oxide surface; a diphenylamine unit (blue) that act as the electron-donating portion of the dye; a thiophene (purple) that links the donor and acceptor units together, helps the dye absorb more light, and contains the recombination-blocking hexyl chains; and a diethylthiobarbituric group (red) that acts as the dye's electron acceptor. The crucial step of the synthesis involves forming the C – N bond between the diphenylamine and the thiophene. The bond is highlighted in orange.

The crucial step in the synthesis of this dye is the formation of the C–N bond (highlighted in orange) between the diphenylamine donor and the thiophene linker. This bond is not found in many other organic dyes, and, to the authors' knowledge, not in any other p-type dyes.

The original synthesis scheme is shown in Figure 5. In this scheme, the dye has a single-anchor, double-acceptor design. A study by our lab (Beauchamp and Click et al.) showed that this design both requires fewer synthetic steps and increases the molar extinction coefficient of the dye by including twice as many light-absorbing dye "arms"[12]. In accordance with the synthesis outlined in that paper, this initial synthesis scheme planned for the dye arms to be completely synthesized before they are attached to the amine containing the anchoring group.

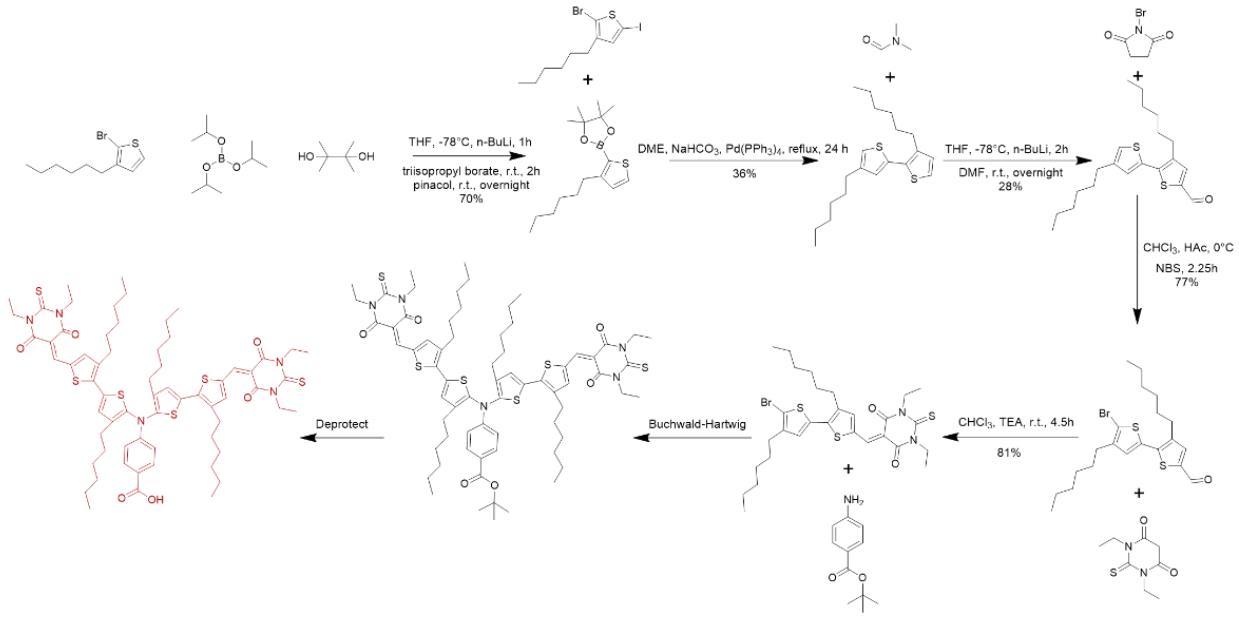


Figure 5. Initial synthesis scheme.

The dye arms (Figure 6, thiophene 1) were successfully synthesized, but the penultimate step (the formation of the C–N bond) was unsuccessful. It was hypothesized that the multitude of functionalizations on the dye arms were hindering the reaction, so test reactions were continued with a simpler (and less synthesis-intensive) thiophene reactant, 5'-bromo-3,4'-dihexyl-2,2'-bithiophene (Figure 6, thiophene 2).

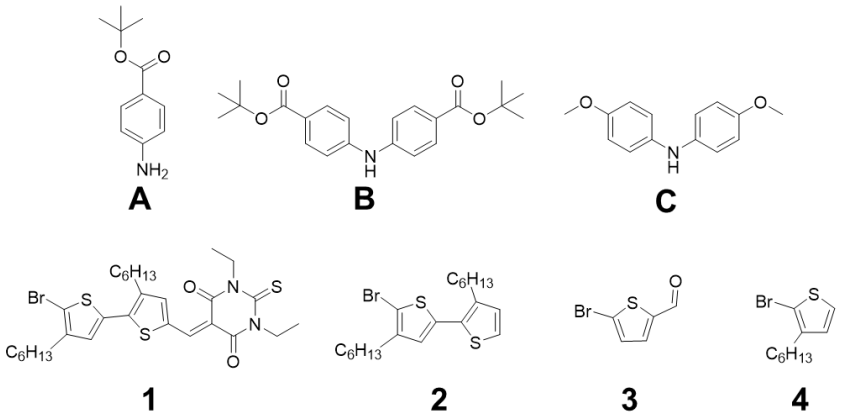


Figure 6. All diphenylamines (top) and thiophenes (bottom) used in preliminary C – N coupling studies.

Using bithiophene as the thiophene reactant was mildly successful. Buchwald-Hartwig conditions using palladium acetate catalyst, several equivalents of tri-tert-butylphosphine ligand, and sodium tert-butoxide base produced over a 37% yield of mono-substituted product (one dye arm attached, but the other did not). The mono-substituted product was isolated and a similar reaction was set up in an attempt to attach the second dye arm. No products or mono-substituted starting material were detected by ESI-MS, indicating that this reaction destroys the starting material.

Since the first reaction using the bithiophene starting material had indicated that it was possible to couple a single dye arm to the amine, the possibility of successfully synthesizing a single-arm dye encouraged us to simplify the synthesis scheme and dye design to a double-anchor, single-acceptor model. A protected diphenylamine (di-tert-butyl 4,4'-azanediyldibenzoate; amine B) was synthesized. This specific diphenylamine was chosen because the tert-butyl ester group can easily be deprotected into the carboxylic acid groups that anchor the dye to the semiconductor surface. We attempted to couple this diphenylamine to the bithiophene under conditions that were similar to a literature procedure that coupled a different diphenylamine (Figure 6, amine C) to a hexylthiophene (thiophene 4) in 64% yield[13]. The failure of this reaction prompted us to eliminate the hexyl chain from the thiophene reactant, removing all possible factors that could get in the way of the 2-position on the thiophene and keep the C–N bond from forming.

In the step after the Buchwald-Hartwig reaction in this revised scheme (Figure 7A), the Knoevenagel condensation attaches the electron accepting portion of the dye. This reaction requires the thiophene to have an carbonyl (in this case, an aldehyde) available for the deprotonated acceptor to attack. Past experiments indicated that forming the aldehyde on the thiophene after attaching it to the diphenylamine would be a difficult and low-yield reaction; therefore, it is more efficient to use a commercially available compound with the aldehyde handle already attached. We chose 5-bromo-2-thiophenecarbaldehyde (Figure 6, thiophene 3), the simplest thiophene meeting the requirements for the Buchwald-Hartwig (halogenated) and the Knoevenagel (carbonyl-containing) as the thiophene in this scheme's Buchwald-Hartwig reaction. Though this newly revised dye design (Figure 7A, red) excludes hexyl chains, it acts as a model dye that could easily be expanded into the ideal dye that incorporates both the protective hexyl chains and the optimal four-thiophene-long π-linker[12].

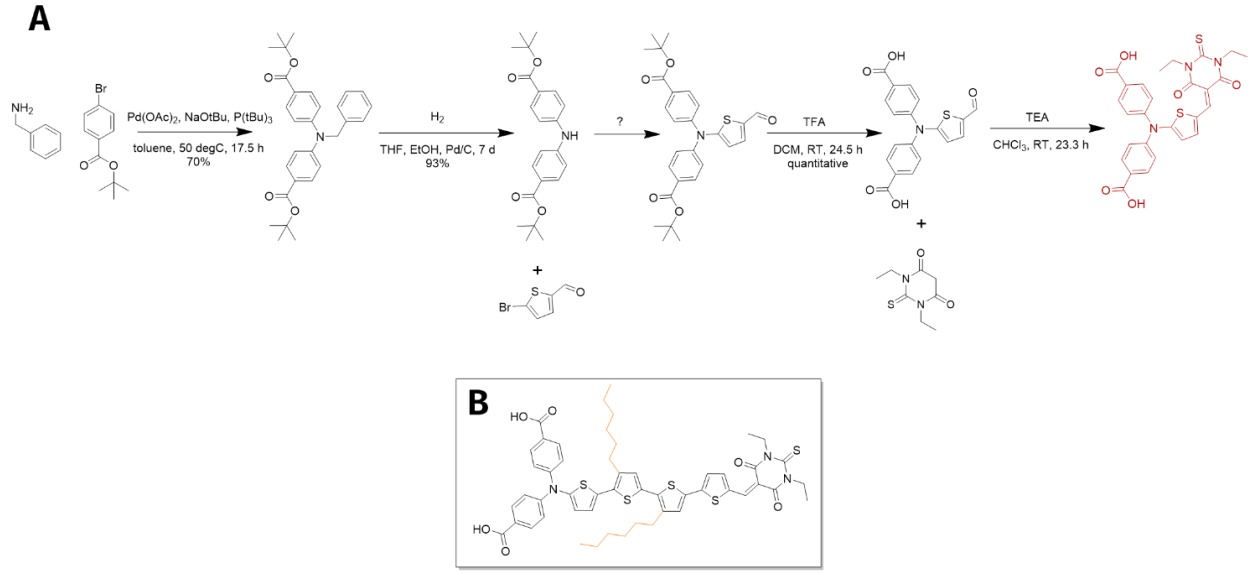


Figure 7. A) Current design (highlighted in red) and synthesis for single-acceptor model dye design. B. Eventual target dye that incorporates four thiophenes (the optimal number of thiophene linkers[12]) as well as the recombination-blocking hexyl chains (highlighted in orange)

Several reactions between the protected diphenylamine (amine B) and the bromothiophenecarbaldehyde (thiophene 3) were run with varying catalysts, ligands, temperatures, and Pd:ligand ratios as suggested by various literature on Buchwald-Hartwig reactions[14–16]. None of

these reactions were successful; if they did produce the desired product, the product was only in yield of 11% or less.

The preliminary work on this project indicates that the C – N bond-formation is the difficult, crucial reaction in this synthesis. Determining which reactants will successfully couple will determine the ultimate structure of the dye and its performance.

TASKS:

Task 1: Determining conditions for successful C–N bond formation between thiophenes and diphenylamines. We plan to vary the functionalizations on the para positions of the diphenylamine to investigate the electronic conditions needed for this reaction.

Beyond determining the specific sets of conditions and reactants needed for the C–N bond to form, the bond formation will be investigated and optimized across reaction types. While the Buchwald-Hartwig is a very powerful reaction, it uses expensive and air-sensitive palladium catalysts and exotic, phosphine-based ligands. There are other possibilities for forming the C–N bond in a manner more conducive to industrial scale-up: the Ullman-type reaction usually is run at higher temperatures but uses cheaper, more-abundant copper catalysts. The Chan-Lam reaction is run with a copper catalyst at moderate or room temperatures in air. All three synthetic routes will be investigated and evaluated in terms of performance and practicality.

Not only will this study discern important synthetic information about the conditions needed for C–N bonds between amines and thiophenes to form, finding the most resource- and cost-effective method will help translate the dye to industrial contexts in the future.

Task 2: Synthesize and characterize entire dye. A shorter dye synthesis saves time, money, and resources for both the lab scientist and the industrial chemical engineer. By finding the shortest pathway for synthesizing a high yield of dye, we improve the scale-up process of industrially manufacturing the dye.

The dye will be synthesized using conventional organic synthesis methods and purified using inexpensive and green, non-resource-intensive methods such as distillation and recrystallization when possible. After synthesizing the dye, we plan to characterize its physical properties by 1HNMR, 13CNMR, mass spectrometry, UV-vis and fluorescence spectroscopy, and cyclic voltammetry.

Task 3: Device testing and optimization. P-type electrodes will be fabricated using doctor-bladed nanoparticle ITO films. Both the dye under consideration as well as a control version of the dye (with the triphenylamine moiety instead of the modified diphenylamine-thiophene structure) will be used to sensitize the films. Using simulated AM1.5 solar illumination, we will measure the solar cells' short-circuit photocurrent, the open-circuit photovoltage, the fill factor, and thus the energy conversion efficiency. If the solar cells' currents are sufficiently high, we plan to fabricate a tandem solar cell with a Z907-sensitized TiO_2 photoanode.

TIMELINE:

Year 1: Investigation of C–N bond forming conditions

Year 2: Synthesis of dye, characterization of dye molecule properties; device fabrication, testing, and optimization

BROADER IMPACT:

Education of undergraduates and graduate students: This project is intended for a graduate-undergraduate student pair. The undergraduate will take charge of the project, learning the research process, synthetic skills, literature searches, experiment design, device fabrication, device characterization, and data analysis. Meanwhile, the graduate student will learn mentorship skills, cultivating leadership, teaching, and research-planning skills essential to their success after graduation. The undergraduate will also undergo thorough training in scientific communication by presenting the results of their research in group meeting and poster presentations as well as preparing a manuscript. Undergraduates become far more equipped to carry out quality research later in their careers when they are active and involved in the entire research process, and advising an undergraduate on an independent project is a useful way for graduate students to learn how to think about and lead projects other than their own.

Our group seeks to mentor and establish strong female researchers. We currently have two talented and motivated undergraduate women working in our lab: Maneesha Pimplikar (class of 2016 chemistry major) and Brittany Trang (class of 2017 chemistry and English major). Maneesha works on synthesizing and characterizing $MoO(S_2)_2$bpy derivatives; Brittany has been working under the guidance of graduate student Kevin Click on the preliminary work for the proposed project. Besides laying the groundwork for this preliminary project, she has secured a small scholarship from Ohio State's Undergraduate Research Office for a second dye project and has also conducted summer research in Germany under the DAAD RISE internship program. Kevin has worked extensively on the synthesis and device characterization organic p-type dyes and dye-sensitized solar cells[6,12]. He has been an excellent mentor so far, independently training Brittany to do organic synthesis when she was still a freshman and supporting her applications for funding and internships.

References

(1) Nazeeruddin, M. K.; Péchy, P.; Grätzel, M. *Chem. Commun.* **1997**, *4* (18), 1705–1706.

(2) Green, M. A.; Emery, K.; Hishikawa, Y.; Warta, W.; Dunlop, E. D. *Prog. Photovoltaics Res. Appl.* **2016**, *24* (7), 905–913.

(3) Komiya R, Fukui A, Murofushi N, Koide N, Yamanaka R, K. H. In *Technical Digest, 21st International Photovoltaic Science and Engineering Conference*; Fukuoka, 2011.

(4) Yella, A.; Lee, H.-W.; Tsao, H. N.; Yi, C.; Chandiran, A. K.; Nazeeruddin, M. K.; Diau, E. W.-G.; Yeh, C.-Y.; Zakeeruddin, S. M.; Grätzel, M. *Science (80-.).* **2011**, *334* (6056), 629–634.

(5) Perera, I. R.; Daeneke, T.; Makuta, S.; Yu, Z.; Tachibana, Y.; Mishra, A.; Bäuerle, P.; Ohlin, C. A.; Bach, U.; Spiccia, L. *Angew. Chemie* **2015**, *127* (12), 3829–3833.

(6) Huang, Z.; He, M.; Yu, M.; Click, K.; Beauchamp, D.; Wu, Y. *Angew. Chemie Int. Ed.* **2015**, *54* (23), 6961–6965.

(7) Wang, Z.-S.; Koumura, N.; Cui, Y.; Takahashi, M.; Sekiguchi, H.; Mori, A.; Kubo, T.; Furube, A.; Hara, K. *Chem. Mater.* **2008**, *20* (12), 3993–4003.

(8) Nattestad, A.; Mozer, A. J.; Fischer, M. K. R.; Cheng, Y.-B.; Mishra, A.; Bäuerle, P.; Bach, U. *Nat. Mater.* **2010**, *9* (1), 31–35.

(9) Gupta, A.; Armel, V.; Xiang, W.; Fanchini, G.; Watkins, S. E.; MacFarlane, D. R.; Bach, U.; Evans, R. A. *Tetrahedron* **2013**, *69* (17), 3584–3592.

(10) Chang, Y. J.; Chow, T. J. *Tetrahedron* **2009**, *65* (24), 4726–4734.

(11) Hagfeldt, A.; Boschloo, G.; Sun, L.; Kloo, L.; Pettersson, H. *Chem. Rev.* **2010**, *110* (11), 6595–6663.

(12) Beauchamp, D. R.; Click, K. A.; Garrett, B. R.; Huang, Z.; Hadad, C. M.; Wu, Y. *Phys. Chem. Chem. Phys.* **2014**.

(13) Gupta, A.; Kelson, M.; Armel, V.; Xiang, W.; Bilic, A.; Bhosale, S. V. *Synth. Met.* **2014**, *193*, 102–109.

(14) Hartwig, J. F.; Kawatsura, M.; Hauck, S. I.; Shaughnessy, K. H.; Alcazar-Roman, L. M. *J. Org. Chem.* **1999**, *64* (15), 5575–5580.

(15) Yamamoto, T.; Nishiyama, M.; Koie, Y. *Tetrahedron Lett.* **1998**, *39* (16), 2367–2370.

(16) Borojeni, S. B. Studies on the Optimization of Buchwald-Hartwig Amination of Aryl Halides, Queen's University, 2014.

Graphical Abstract/Table of Contents (TOC) Image

The graphical abstract is a visual version of a scientific article's abstract; it visually summarizes the important point of a paper. Journal websites display them in the results of a search or in the list of articles in an issue.

As a researcher, I often judge whether I want to read a paper by its TOC. I most commonly encounter them when I follow a reference from another paper and find the homepage for another article. The TOC gives me clues as to what field the paper is from (analytical, organic, and materials papers on the same subject will emphasize different facets of the problem though the graphical abstract) and whether the content is relevant to my interests.

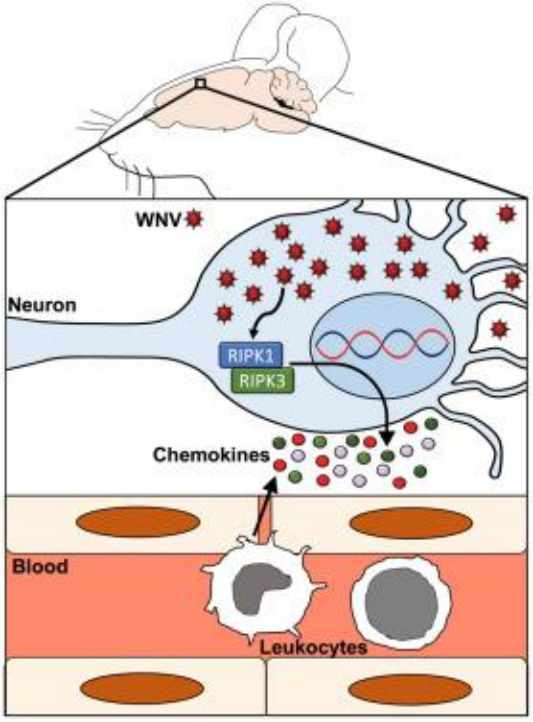
Cell Press' guidelines for graphical abstracts are among the most detailed and helpful. The publisher stresses the importance of expressing ideas in a visual form instead of with graphs or data. It also specifies many criteria for making the image easy to follow and visually pleasing.

However, biological processes are usually more visual than chemical processes. The TOC guidelines for the Journal of the American Chemical Society have far fewer stipulations about the making the image visually appealing. It essentially only requires that the authors avoid using long sentences and elements that are already contained within the manuscript. I have included several examples of graphical abstracts from biological and chemical journals below.

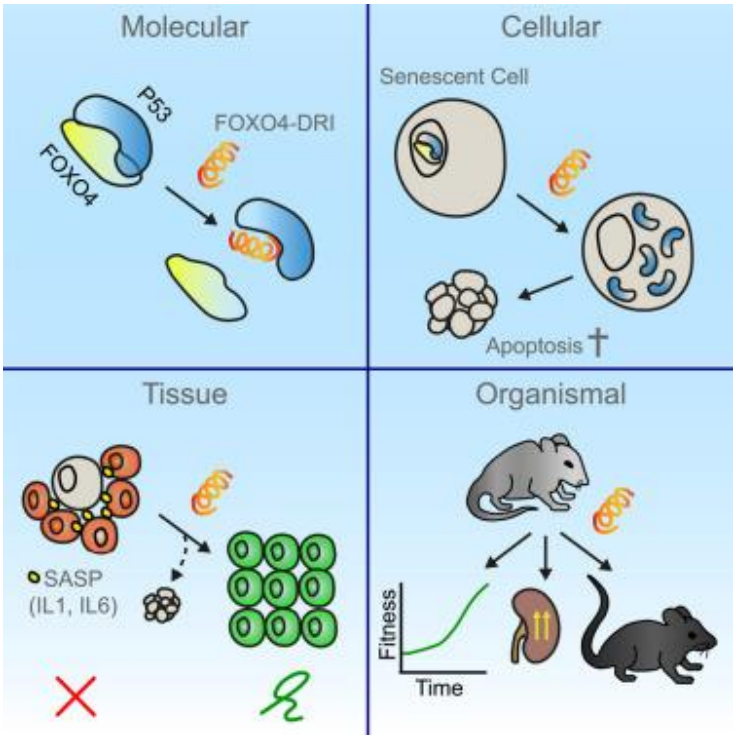
While norming against TOC images from articles written about dye-sensitized solar cells (several examples included in the Resources section), I found that many were subpar in the "visually interesting" category. Most included the structure of the dye and a sometimes graph, which gets the point across to someone in the field but is not visually attractive. These kinds of images also only illustrates one point: "We made this and it does this."

In my TOC image, I attempt to show the dye, the results, and also the principles behind the study that make the results so exciting: that changing the dye's structure from a nitrogen bonded to a phenyl to a nitrogen bonded to a hexylthiophene has a profound effect on the dye's electronic levels and current production. This image incorporates a large portion of the study into a single and relatively attractive image.

Examples of graphical abstracts from biological journals:

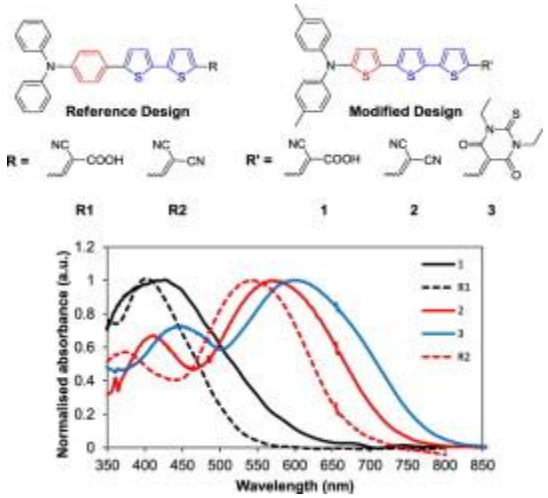


"RIPK3 Restricts Viral Pathogenesis via Cell Death-Independent Neuroinflammation" (Daniels et al.)

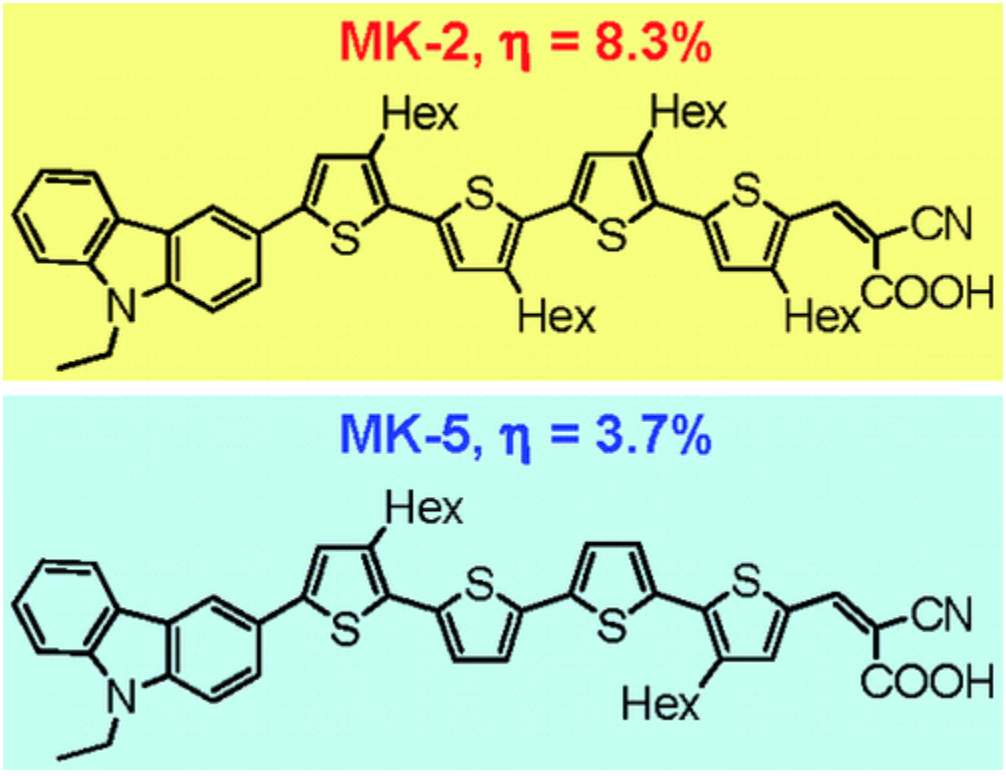


"Targeted Apoptosis of Senescent Cells Restores Tissue Homeostasis in Response to Chemotoxicity and Aging" (Baar et al.)

Examples of TOC images for dye-sensitized solar cell papers from chemistry journals:



"The effect of direct amine substituted push–pull oligothiophene chromophores on dye-sensitized and bulk heterojunction solar cells performance" (Gupta et al.)



"Hexylthiophene-Functionalized Carbazole Dyes for Efficient Molecular Photovoltaics: Tuning of Solar-Cell Performance by Structural Modification" (Wang et al.)

Resources:

"Cell Press Graphical Abstract Guidelines." *Cell Press*, www.cell.com/pb/assets/raw/shared/figureguidelines/GA_guide.pdf. 9 April 2016.

"Guidelines for Table of Contents/Abstract Graphics." *ACS Publications*, 17 February 2017, pubs.acs.org/paragonplus/submission/toc_abstract_graphics_guidelines.pdf. 9 April 2016.

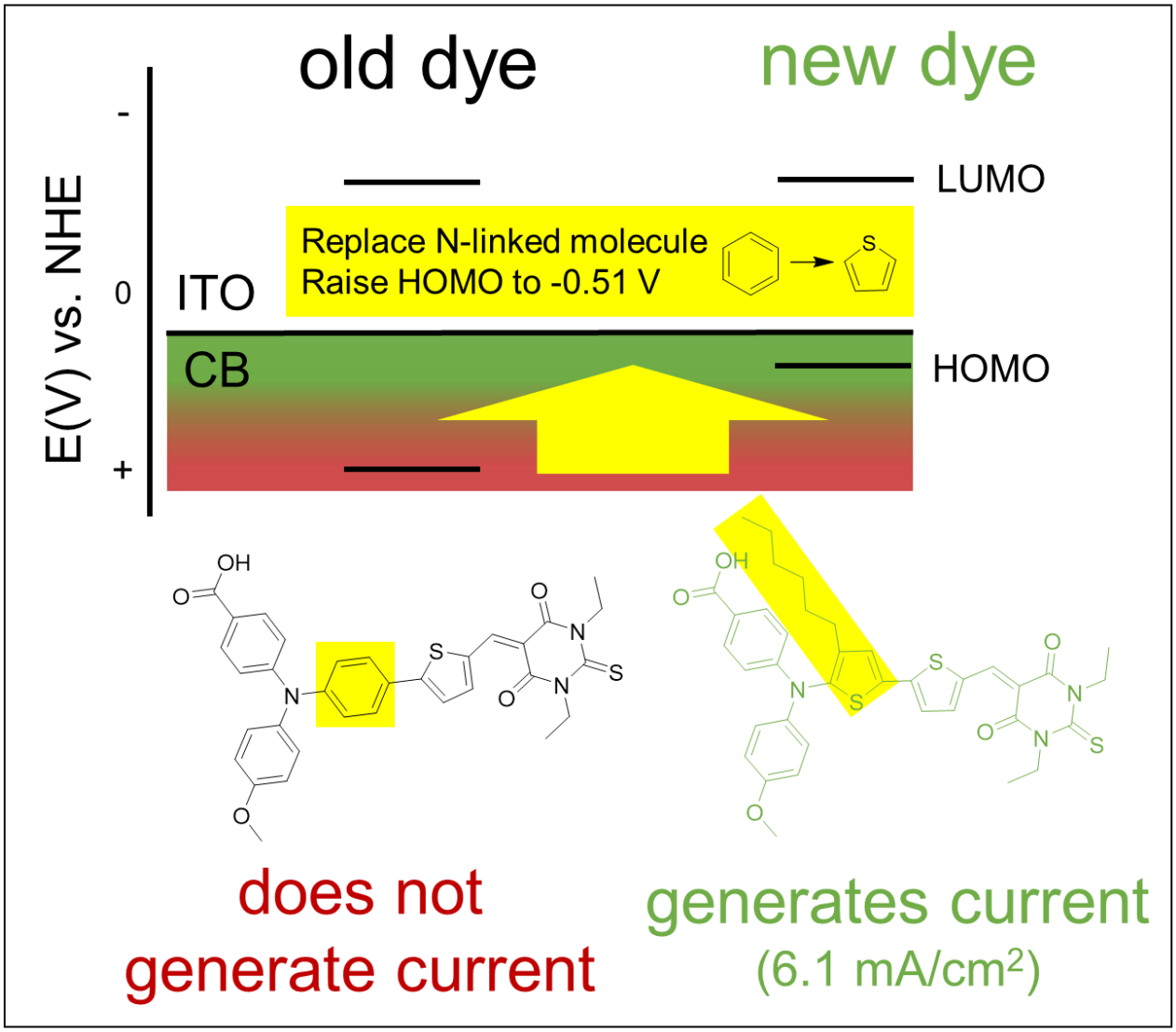
Articles and graphical abstracts used for norming:

Baar, Marjolein P. et al. "Targeted Apoptosis of Senescent Cells Restores Tissue Homeostasis in Response to Chemotoxicity and Aging." Cell 169.1 (2017): 132–147.e16. Web. 9 Apr. 2017.

Daniels, Brian P. et al. "RIPK3 Restricts Viral Pathogenesis via Cell Death-Independent Neuroinflammation." Cell 169.2 (2017): 301–313.e11. Web. 9 Apr. 2017.

Gupta, Akhil et al. "The Effect of Direct Amine Substituted Push–pull Oligothiophene Chromophores on Dye-Sensitized and Bulk Heterojunction Solar Cells Performance." Tetrahedron 69.17 (2013): 3584–3592. Web. 20 Nov. 2014.

Wang, Zhong-Sheng et al. "Hexylthiophene-Functionalized Carbazole Dyes for Efficient Molecular Photovoltaics: Tuning of Solar-Cell Performance by Structural Modification." Chemistry of Materials 20.12 (2008): 3993–4003. Web. 22 Feb. 2016.


old dye
new dye
E(V) vs. NHE
-
0
+
ITO
CB
LUMO
HOMO
Replace N-linked molecule
Raise HOMO to -0.51 V
S
OH
O
N
S
O
N
S
O
N
S
does not
generate current
generates current
(6.1 mA/cm2)